

Liquid Phase Behavior of Ionic Liquids with Alcohols: Experimental Studies and Modeling

J.M. Crosthwaite, M.J. Muldoon, S.N.V.K Aki, E.J. Maginn, and J.F. Brennecke^{C,S}

*Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN, U.S.A.
jfb@nd.edu*

Ionic liquids (ILs) have been suggested as potential “green” solvents to replace volatile organic solvents in reaction and separation processes due to their negligible vapor pressure. In order to develop ILs for these applications, it is important to gain a fundamental understanding of the factors that control the phase behavior of ionic liquids with other liquids. In this work, we continue our study of the effect of different factors on the phase behavior of ionic liquids with alcohols, focusing on pyridinium ILs for comparison with imidazolium ILs from our previous studies. The impact of different alcohol and IL characteristics, including alcohol chain length, cation alkyl chain length, anion, different substituent groups on the pyridinium cation, and the type of cation (pyridinium vs. imidazolium), will be discussed. In general, the same type of behavior is observed for pyridinium and imidazolium ILs, with all systems studied exhibiting upper critical solution temperature behavior. The impact of alcohol chain length, cation chain length, and anion are the same for pyridinium ILs as those observed previously for imidazolium ILs. However, the effect of the cation type on the phase behavior is dependent on the strength of the cation-anion interaction. Additionally, all systems from this study and also from our previous work for imidazolium ILs were modeled using the Non-Random Two Liquid (NRTL) equation using two different approaches for determining the adjustable parameters. For all systems, the NRTL equation with binary interaction parameters and a linear temperature dependence provided a good fit of the experimental data.